

A Compact Approximate Solution to the Kondo Problem

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Abstract

A compact approximate groundstate of the Kondo problem is introduced. It consists of four Slater states. The spin up and down states of the localized d-impurity are paired with two localized s-electron states of opposite spin. All the remaining s-electron states are rearranged forming two new optimal orthonormal bases. Through a rotation in Hilbert space the two localized states (and the rest of the bases) are optimized by minimizing the energy expectation value. The ground-state energy E_0 and the singlet-triplet excitation energy ΔE_{st} are calculated numerically. Although the two energies can differ by a factor of 1000, they are obtained simultaneously. The singlet-triplet excitation energy ΔE_{st} is proportional to $\exp[-1/2J\rho]$ and quite close to the Kondo temperature $k_B T_K$. The cases for anti-ferromagnetic ($J > 0$) and ferromagnetic ($J < 0$) coupling are investigated.

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1 Introduction

The properties of magnetic impurities in a metal is one of the most intensively studied problems in solid state physics. The work of Friedel [1] and Anderson

[2] laid the foundation to understand why some transition-metal impurities form a local magnetic moment while others don't. Kondo [3] showed that multiple scattering of conduction electrons by a magnetic impurity yields a divergent contribution to the resistance in perturbation theory. In the following three decades a large number of sophisticated methods were applied to better understand and solve the Kondo model, and it was shown that at zero temperature a Kondo impurity is in a non-magnetic state. To name a few of these methods: scaling [4], renormalization [5], [6], Fermi-liquid theory [7], [8], slave-bosons (see for example [9]), and the Bethe-ansatz [10], [11]. For a review see [12]. For numerical calculation an approximate wave function by Varma and Yafet [13] which was later extended to the large-spin limit [14], [15] was particularly productive. Finally after decades of research exact solutions of the Kondo and Friedel-Anderson problems were derived [10], [16].

One of the authors [17], [18] recently introduced a new approach to the Friedel-Anderson impurity. This approach is based on building from the s-electron spectrum a localized s-state for each spin which behaves as an artificial Friedel resonance (AFR) states. This permits the construction of a very compact approximate ground state (see appendix, equ. (2)). It requires solely the optimization of the two localized AFR states and consists of a few Slater states (Slater determinants). This solution gives remarkably good results for the ground-state energies and the occupation of the d-states. The results are of the same quality as numerical calculation by Gunnarsson and Schoenhammer [19] who applied the large N_f method to the spin 1/2 Friedel-Anderson model and included self-consistently up to 10^7 basis states.

In this paper we introduce a similar ansatz to the Kondo effect. The intension is to rederive some of the well known properties of the Kondo effect within a rather simple and transparent frame work. The hope is to extend this rather simple method to more complex problems such as the interaction between Kondo impurities.

2 The AFR-Groundstate for the Kondo Effect

The Kondo ground state which is suggested in this paper is derived from the Friedel resonance problem. Below equation (2) gives the Friedel-Anderson

Hamiltonian. If one removes the Coulomb exchange interaction term $Un_{d+}n_{d-}$ then one obtains the Hamiltonian for the Friedel resonance. This is a single-particle Hamiltonian and the n -electron ground state can be written as a simple product of single electron states which are a hybridization of the d-electrons with the band s-electrons.

Due to the s-d-interaction between the s-electrons and the d-impurity the s-electrons shift their weight towards the d-impurity. This is more clearly expressed in a different version of the n -electron ground state of the Friedel impurity [20]. The system forms from the s-band a state a_0^* which is localized in the close vicinity of the d^* -state. This a_0^* -state hybridizes with the d^* -state in the form $(Aa_0^* + Bd^*)$, where A, B are coefficients. The remaining s-electrons are arranged in states a_i^* ($1 \leq i \leq N-1$) which are orthogonal to a_0^* and each other. (Furthermore the matrix elements of the free electron Hamiltonian H_0 must be diagonal $\langle a_i^* \Phi_0 | H_0 | a_j^* \Phi_0 \rangle = E(i) \delta_{ij}$ for $i, j \geq 1$, see appendix). Then the alternative version of the $(n+1)$ -electron Friedel ground state is given by

$$\psi_{Fr} = (Aa_0^* + Bd^*) |\mathbf{0}_a\rangle \quad (1)$$

where the hybrid $(Aa_0^* + Bd^*)$ plus the n lowest states $a_1^* a_2^* \dots a_n^* = |\mathbf{0}_a\rangle$ of the basis $\{a_i^*\}$ are occupied. The state a_0^* can be found by numerical variation or from an analytic expression (from a_0^* the full basis $\{a_i^*\}$ can be derived). One of the authors has proved [21] that (1) is an exact ground state of the Friedel impurity.

In the next step we consider the Friedel-Anderson impurity whose Hamiltonian is given in equ. (2).

$$H_{FA} = \sum_{\sigma} \left\{ \sum_{\nu=1}^N \varepsilon_{\nu} c_{\nu\sigma}^* c_{\nu\sigma} + E_d d_{\sigma}^* d_{\sigma} + \sum_{\nu=1}^N V_{sd}(\nu) [d_{\sigma}^* c_{\nu\sigma} + c_{\nu\sigma}^* d_{\sigma}] \right\} + Un_{d+}n_{d-} \quad (2)$$

Its mean field solution is just a product of two Friedel solutions as given by equ. (1), one for the spin up and the other for the spin down electrons (with different effective d^* -state energies $E_{d\uparrow}$ and $E_{d\downarrow}$). It requires two localized s-states, which we denote now as a_0^* for spin up and b_0^* for spin down and the rest of their bases $\{a_i^*\}$ and $\{b_i^*\}$. The two differ when the impurity is magnetic.

The mean field solution can be dramatically improved if one expands the product of the two hybridized states $(A_{\uparrow} a_{0\uparrow}^* + B_{\uparrow} d_{\uparrow}^*) (A_{\downarrow} b_{0\downarrow}^* + B_{\downarrow} d_{\downarrow}^*)$ and assigns new coefficients (A, B, C, D) for four two-electron states. This yields

$$\psi_{ms} = [Aa_{0\uparrow}^* b_{0\downarrow}^* + Ba_{0\uparrow}^* d_{\downarrow}^* + Cd_{\uparrow}^* b_{0\downarrow}^* + Dd_{\uparrow}^* d_{\downarrow}^*] |\mathbf{0}_{a\uparrow}\rangle |\mathbf{0}_{b\downarrow}\rangle \quad (3)$$

The optimal state ψ_{ms} is obtained by varying the composition of a_0^* and b_0^* and optimizing the coefficients (A, B, C, D) . This solution has the same structure as the mean field solution but it yields a much lower ground-state energy. It also requires a much larger threshold Coulomb exchange energy U to form a magnetic moment at the impurity.

The study of the Kondo effect taught us that the real ground state of the Friedel-Anderson impurity is a symmetric state (often called a singlet state). Such a state can be constructed from (3) by reversing the spins of all electrons and combining the two states. This yields

$$\begin{aligned} \psi_{ss} = & [Aa_{0\uparrow}^* b_{0\downarrow}^* + Ba_{0\uparrow}^* d_{\downarrow}^* + Cd_{\uparrow}^* b_{0\downarrow}^* + Dd_{\uparrow}^* d_{\downarrow}^*] |\mathbf{0}_{a\uparrow}\rangle |\mathbf{0}_{b\downarrow}\rangle \\ & + [A'b_{0\uparrow}^* a_{0\downarrow}^* + C'b_{0\uparrow}^* d_{\downarrow}^* + Bd_{\uparrow}^* a_{0\downarrow}^* + D'd_{\uparrow}^* d_{\downarrow}^*] |\mathbf{0}_{b\uparrow}\rangle |\mathbf{0}_{a\downarrow}\rangle \end{aligned} \quad (4)$$

In equ. (4) the creation operators have been reordered according to their spin. By optimizing the localized states and the coefficients we obtained an almost perfect agreement with Gunnarsson and Schoenhammer [19] for the ground-state energy and the zero, single and double occupation of the d^* -state.

In this paper we are interested in the Kondo effect. For the treatment of a magnetic impurity Kondo used the exchange Hamiltonian H_{sd} with the exchange interaction $J_{\mathbf{k},\mathbf{k}'}$. One generally approximates the exchange interaction by a $\delta(\mathbf{r})$ -function: $J(\mathbf{r}) = v_a \delta(\mathbf{r})$ where v_a is atomic volume. Then the exchange (or Kondo) Hamiltonian has the form

$$H_{sd} = v_a J \left[\begin{aligned} & \left(S_+ \Psi_{\downarrow}^{\dagger}(0) \Psi_{\uparrow}(0) + S_- \Psi_{\uparrow}^{\dagger}(0) \Psi_{\downarrow}(0) \right) \\ & + S_z \left(\Psi_{\uparrow}^{\dagger}(0) \Psi_{\uparrow}(0) - \Psi_{\downarrow}^{\dagger}(0) \Psi_{\downarrow}(0) \right) \end{aligned} \right] \quad (5)$$

where S_+ , S_- , S_z are the spin operators of the impurity with spin $S = 1/2$ and $\Psi_{\uparrow}^{\dagger}(0)$ and $\Psi_{\downarrow}^{\dagger}(0)$ represent field operators. The product $v_a J \Psi_{\sigma}^{\dagger}(0) \Psi_{\sigma'}(0)$ yields an energy since $\Psi_{\sigma}^{\dagger}(0) \Psi_{\sigma'}(0)$ has the dimension of a density.

Schrieffer and Wolff [22] showed that there is an intimate connection between the Friedel-Anderson and the Kondo impurity. The Friedel-Anderson Hamiltonian can be transformed into an exchange Hamiltonian with an anti-ferromagnetic exchange interaction $J > 0$ (plus some additional terms). In particular for large values of U and large negative E_d (for example $E_d = -U$)

they derived an effective J

$$J \approx -|V_{sd}|^2 \frac{U}{(U + E_d) E_d} > 0 \quad (6)$$

The Kondo impurity is in some respects a limiting case of the Friedel-Anderson impurity. By increasing the exchange interaction U (and decreasing $E_d = -U/2$) the Friedel-Anderson impurity approaches the properties of a Kondo impurity. For the Kondo impurity the d-impurity is a localized permanent magnetic moment. This means that the d^* -state is always singly occupied, either with spin up or down. We observe this transition in our solution ψ_{ss} (equ. 4). When we increase U (with $E_d = -U/2$) the coefficients A, A' and D, D' approach zero. It becomes energetically too expensive to have an empty or doubly occupied d^* -state. Therefore for the Kondo impurity we make the following ansatz for the ground state

$$\begin{aligned} \psi_K &= (Ba_{0\uparrow}^*d_{\downarrow}^* + Cd_{\uparrow}^*b_{0\downarrow}^*)|\mathbf{0}_{a\uparrow}\mathbf{0}_{b\downarrow}\rangle + (\overline{C}b_{0\uparrow}^*d_{\downarrow}^* + \overline{B}d_{\uparrow}^*a_{0\downarrow}^*)|\mathbf{0}_{b\uparrow}\mathbf{0}_{a\downarrow}\rangle \\ &= B\psi_B + C\psi_C + \overline{C}\psi_{\overline{C}} + \overline{B}\psi_{\overline{B}} \end{aligned} \quad (7)$$

We remove the terms with zero and double d-occupancy from the AF ground state ψ_{ss} .

We denote the state ψ_K as the **AFR ground state** of the Kondo effect since it uses the artificial Friedel resonance states a_0^* and b_0^* .

As in the AF ground state ψ_{ss} the states a_0^* and b_0^* are localized s-states which are concentrated close to the impurity. Their composition will be numerically optimized. Here, we sketch briefly the construction of the $\{a_0^*, a_i^*\}$ basis. (The construction of the $\{b_0^*, b_i^*\}$ is completely analogous).

In this paper we use a finite s-electron band with N states c_ν^* per spin and a magnetic d^* -state with spin $S = 1/2$. For the present calculations we use Wilson's band which extends from -1 to $+1$ and has an exponentially fine energy spectrum close to the Fermi energy (see appendix). The a_0^* -state is composed of these c_ν^* -states

$$a_0^* = \sum_{\nu=1}^N \alpha_\nu^* c_\nu^* \quad (8)$$

(In the initial phase the coefficients α_ν^* are arbitrarily chosen, for example being constant).

The remaining s-electron basis $\{c_\nu^*\}$ has to be made orthogonal to a_0^* . This yields the new remaining bases $\{a_i^*\}$. The a_i^* ($1 \leq i \leq N-1$) are built

orthogonally to a_0^* and to each other. In addition their $(N - 1) \times (N - 1)$ sub-matrix of the s-band Hamiltonian $H_0 = \sum \varepsilon_\nu n_\nu$ is made diagonal. The a_i^* together with a_0^* represent a new basis. (Details of the construction of the states $\{a_0^*, a_i^*\}$ is discussed in ref. [17], [18] and briefly in the appendix). The states a_i^* are uniquely determined from the state a_0^* . Their form is

$$a_i^* = \sum_{\nu=1}^N \alpha_i^\nu c_\nu^*$$

The new bases $\{a_0^*, a_i^*\}$ can be expressed as a rotation of the original basis $\{c_\nu^*\}$ in Hilbert space. The basis $\{b_0^*, b_i^*\}$ is built in complete analogy.

The free electron Hamiltonian can be expressed in either of the two new bases. It is diagonal in the states a_i^* for $1 \leq i \leq (N - 1)$ and has the form

$$H_0 = \sum_{\nu=1}^N \varepsilon_\nu c_\nu^* c_\nu = \sum_{i=1}^{N-1} E(i) a_i^* a_i + E(0) a_0^* a_0 + \sum_{i=1}^{N-1} V_{fr}^a(i) [a_0^* a_i + a_i^* a_0] \quad (9)$$

The Hamiltonian is equivalent to a Friedel Hamiltonian where a_0^* is an artificial Friedel resonance state (AFR state) which is purely composed of s-states.

After the initial construction of the two bases $\{a_0^*, a_i^*\}$ and $\{b_0^*, b_i^*\}$ the AFR ground state (7) of the Kondo impurity can be formed.

3 Numerical Results

The procedure to obtain the optimal states a_0^* and b_0^* has been described in previous papers [20], [17], [18] and is briefly sketched in the appendix. One starts from an s-band with N states possessing the energy ε_ν . In all calculations the energy band ranges from -1 to 1 following Wilson's example. The density of states is constant and equal to $\rho = 1/2$ (corresponding to one state in the whole band). This band is divided into N adjacent cells $(E_{\nu-1} : E_\nu)$. The energy values in the center (middle) of each cell yield the spectrum $\varepsilon_\nu = (E_\nu - E_{\nu-1}) / 2$.

It was pointed out by Wilson and will be confirmed in the present calculation, that a very small energy spacing δE at the Fermi energy is of essential importance for obtaining the Kondo ground state. A linear energy scale is therefore not well suited for the Kondo ground state because δE is always

much too large. We use an energy spectrum with an exponential energy scale. This energy spectrum was introduced by Wilson [5] in his Kondo paper. Starting with the values of -1 and $+1$ the energy is $N/2$ times divided by 2, yielding the cells $(-1 : -1/2), (-1/2 : -1/4), \dots (-1/2^{N/2} : 0)$. The negative value of ε_ν are (for $1 \leq \nu \leq N/2$): $-3/4, -3/8, \dots, -3/2^{\nu+1}, \dots -3/2^{N/2+1}, -1/2^{N/2+1}$. The positive energies are the mirror image of the negative ones.

From the chosen energy spectrum the two states a_0^* and b_0^* are constructed with initially arbitrary coefficients α_0^ν and β_0^ν . The states a_0^* and b_0^* determine uniquely the full bases $\{a_0^*, a_i^*\}$ and $\{b_0^*, b_i^*\}$ (see appendix). With the two bases the energy matrix elements between the different Slater states are calculated.

The wave function has four components and the Hamiltonian consists of four terms due to H_{sd} and two terms due to H_0 . Therefore the energy expectation value is composed of 96 matrix elements. Many of these are identical and one has to calculate only 16 different matrix elements. They can be transformed into determinants of $(n+1) \times (n+1)$ matrices. In the appendix some representative matrix elements are derived.

Since the two Slater states $(\psi_B, \psi_{\overline{C}})$ are not orthogonal (nor are $(\psi_C, \psi_{\overline{B}})$) one has first to apply an transformation to the four-component basis $(B, \overline{C}, C, \overline{B})^\dagger$ before one can solve the eigenvalue problem. (Details of the optimization are described in the appendix.)

The lowest value of Λ yields the lowest energy expectation value $\langle E \rangle$ for the chosen two bases $\{a_0^*, a_i^*\}$ and $\{b_0^*, b_i^*\}$. Then states a_0^* and b_0^* are rotated in Hilbert space until the value $\langle E \rangle$ reaches a minimum. The resulting state is defined as the AFR ground state of the Kondo impurity and the energy

$E_{00} = \langle E \rangle$ is its ground-state energy.

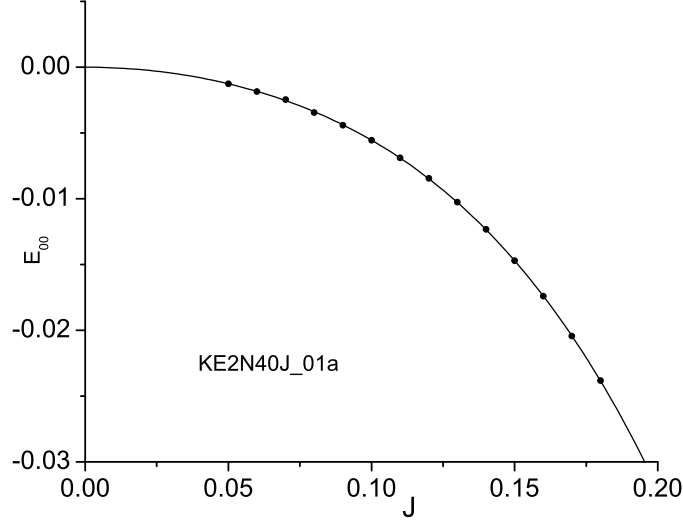


Fig.1: The energy of the AFR ground state of the Kondo impurity as a function of the exchange interaction J for $N = 40$ states.

This ground-state energy E_{00} is plotted in Fig.1 as a function of the exchange interaction J . The curve shows the results for the exponential spectra with $N = 40$. The corresponding value for the energy spacing at the Fermi energy is $\delta E = 1/2^{20} \approx 1 \times 10^{-6}$.

The ground-state energy E_{00} can be well expressed by the following dependence

$$E_{00}(J) = -.5017 * J^2 + .435 * J^3 - 9.65 * J^4$$

This ground-state energy is **not** the Kondo energy. It is sometimes called the perturbational part of the ground-state energy. It is (in most cases) ignored in the Kondo effect as the non-singular part of the ground-state energy. Below we will compare this ground state with the ground-state energy for ferromagnetic coupling, i.e. for negative values of J .

The solution of the eigenvalue equation (14) yields four eigenvalues. The lowest eigenvalue corresponds to the ground-state energy. This should be

a singlet state. We expect that the next eigenvalue of the energy, corresponding to the first excited state, represents a triplet state. To confirm these expectance we calculate the expectation value of the total spin squared $\mathbf{S}^2 = (\sum_i \mathbf{s}_i)^2$ for the two states. For $J = 0.1$ we find in the ground state $\langle \mathbf{S}^2 \rangle = 0.04$. For the first excited state we obtain for the square of the total spin $\langle \mathbf{S}^2 \rangle = 1.99$. This is very close to the value 2 which we expect for $S = 1$. We conclude that the ground state is not a perfect singlet state but is pretty close to it. It is essentially a state with $S = 0$, but it has a small component of a larger total spin such as $S = 1, 2, \dots$. Similarly the first excited state has essentially the total spin $S = 1$. But it too has a small admixture of states with S equal to $0, 2, \dots$ (The fact that $\langle \mathbf{S}^2 \rangle$ is so close to 2 means that the contributions of $S = 0$ and $S = 2$ essentially cancel each other). For the rest of the paper we denote the ground state as the singlet state $\psi_{K,0}$. The first excited state we denote as a triplet state $\psi_{K,1}$.

The energy difference between these two lowest energy states we denote as the singlet-triplet excitation energy ΔE_{st} . This energy difference ΔE_{st} is very small and $\ln(\Delta E_{st})$ is shown in Fig.2 in a logarithmic plot as a function of the inverse coupling strength $1/J$. ΔE_{st} follows an exponential law covering six orders of magnitude in the range $0.05 \leq J \leq 0.18$. The linear full curve in Fig.2 is given by $\Delta E \approx 5 * D * \exp[-x]$ where $x = 1/(2J\rho_0)$. The other data and curves in Fig.2 are explained in the discussion.

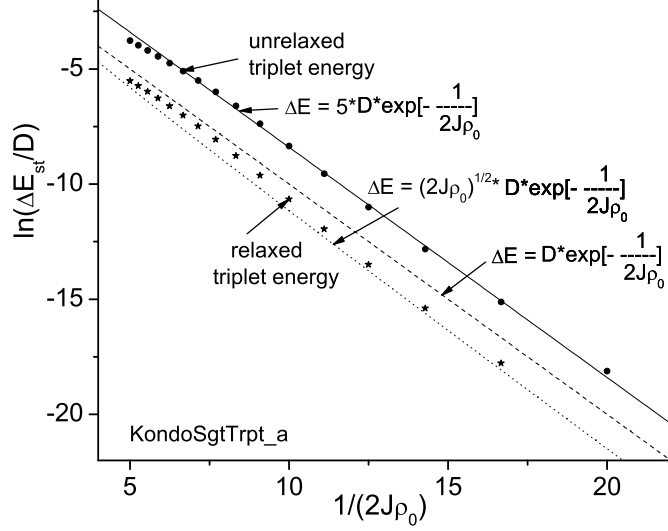


Fig.2: The energy difference between the singlet and triplet state. The full circles are obtained as the energy difference between the ground state and the first excited state. The stars and the dashed and dotted curves are explained in the discussion. A exponential Wilson band with $N = 40$ and $N = 60$ is used in the calculation.

Wilson has shown that the energy separation of the states at the Fermi energy has to be smaller than the Kondo energy to obtain the full Kondo effect (or in Wilson's words: to make the transition into the infinitely strong coupling case). This same behavior is observed in our AFR solution.

We investigate how critical the smallest level separation δE at the Fermi energy is. For this purpose we vary the number N of states for the exponential energy spectrum. The level spacing at the Fermi energy δE depends exponentially on N : $\delta E = 2^{-N/2}$. For each N we calculate the AFR ground state for two values of J , $J = 0.1$ and $J = 0.07$. In Fig.3 the singlet-triplet energy difference ΔE_{st} is plotted versus the smallest energy spacing δE in a log-log plot. The number N of energy levels is varied from $N = 12$ (at the right side) to $N = 48$ (left side). One recognizes that for sufficiently small δE

(on the left side of the figure) the singlet-triplet excitation energy assumes a constant value. With increasing δE the excitation energy increases. The dashed straight line has a slope of 0.85 corresponding to an increase of ΔE_{st} proportional to $(\delta E)^{0.85}$. Fig.3 demonstrates that the transition to a constant ΔE_{st} occurs roughly for $\delta E \approx \Delta E_{st}$ and that δE must be at least a factor 10 smaller than the final result for ΔE_{st} to give a reliable value for ΔE_{st} .

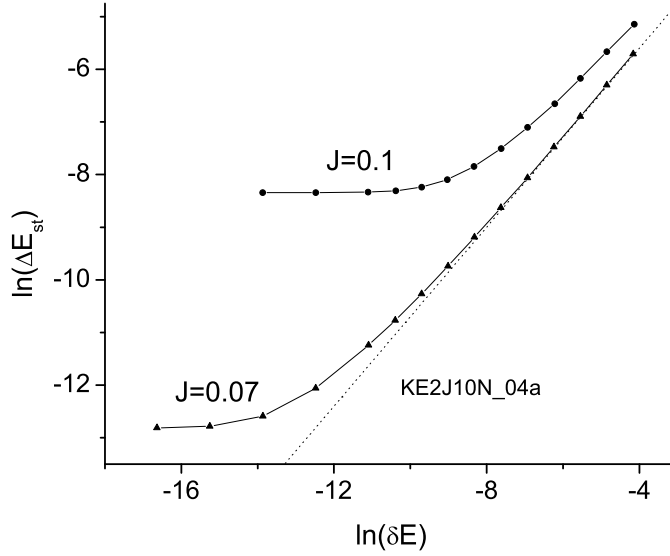


Fig.3: The logarithm of the singlet-triplet excitation energy versus the logarithm of smallest energy spacing δE at the Fermi energy.

3.1 AFR ground state for ferromagnetic coupling

One of the interesting aspects of the exchange Hamiltonian is that it only yields the Kondo anomaly for anti-ferromagnetic coupling or $J > 0$. We apply the AFR-ansatz to the case of ferromagnetic coupling, i.e. $J < 0$. In Fig.4 the resulting ground-state energy is plotted versus the absolute value $|J|$. The ground-state energy lies somewhat above that of the Kondo case with anti-ferromagnetic coupling. The difference is about 10% for small $|J|$ and a factor two for $|J| \approx 0.18$.

It is in particular interesting that the two lowest eigenvalues of equation (14) differ on by about 10^{-11} for sufficiently small level separation δE . Here the value of $|\Delta E_{st}|$ is always much smaller than δE . In other words, at all temperatures the two states, singlet and triplet, are degenerate and the impurity is magnetic. The AFR solutions for anti-ferromagnetic and ferromagnetic coupling are distinctively different.

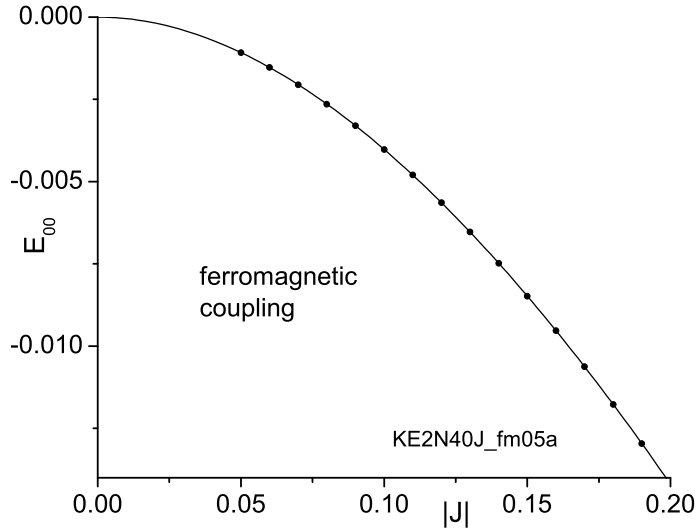


Fig.4: The ground-state energy of the system for negative J , i.e., for ferromagnetic coupling.

$$E_{0mf} = -.4630 * J^2 + .680 * J^3 - .697 * J^4$$

3.2 The artificial Friedel resonance states

3.2.1 Anti-ferromagnetic coupling ($J > 0$)

The whole bases $\{a_0^*, a_i^*\}$ and $\{b_0^*, b_i^*\}$ can be derived from the composition of the AFR states a_0^* and b_0^* . In Fig.5a,b the coefficients α_0^ν and β_0^ν of the states a_0^* and b_0^* are plotted versus the state index ν for $N = 40$ (using equ.(8)). On the left and right side of $\nu = N/2$ the values of ν and $(N - \nu)$

represent essentially the logarithm of the energy. The coefficients are always positive because this yields the maximal interaction of the AFR states with the magnetic d^* state. The state a_0^* is mainly composed of states below ε_F and b_0^* has its main weight at energies above ε_F . However, in the center close to the Fermi energy the amplitudes of the two localized states are essentially identical. This is a behavior which we also observed for the Friedel-Anderson impurity.

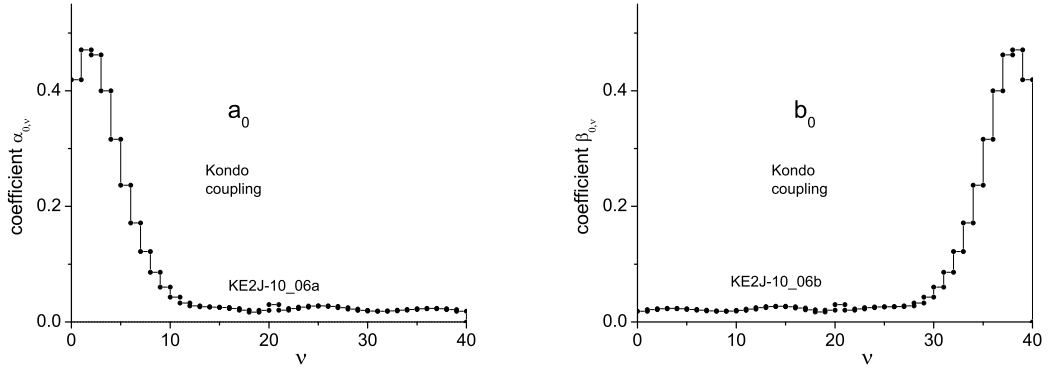


Fig.5a,b: The coefficients of the AFR states α_0^ν and β_0^ν as a function of ν for the two AFR states a_0^* and b_0^* . The exchange interaction is for anti-ferromagnetically coupling ($J = 0.1$).

For large energies the amplitudes α_0^ν and β_0^ν of a_0^* and b_0^* are rather different. For the analysis at small energies we plot the occupation density $|\alpha_0^\nu|^2 / (E_\nu - E_{\nu-1})$ and $|\beta_0^\nu|^2 / (E_\nu - E_{\nu-1})$ as a function of ν . This is shown in Fig.6 where both occupations are plotted in the same figure. At energies

close to the Fermi energy the occupations of a_0^* and b_0^* are almost identical.

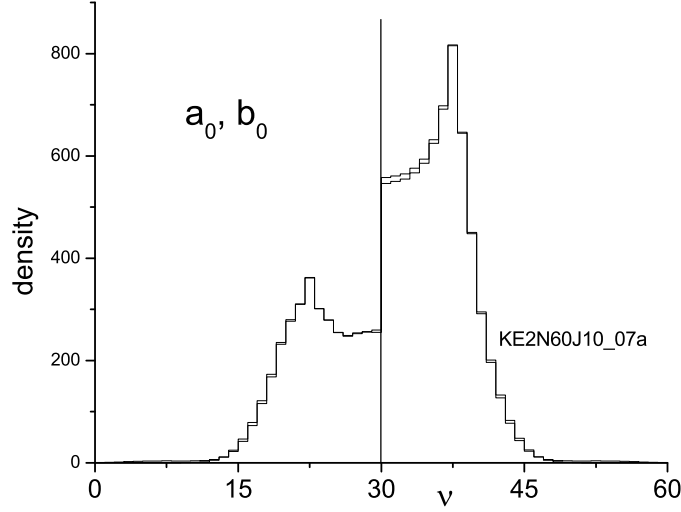


Fig.6: The occupation of the a_0^* and b_0^* AFR states for $N = 60$. Note that the figure shows two curves as a function of ν ($0 \leq \nu \leq 60$). At small energies (close to the center arrow) the two are almost identical.

3.2.2 Ferromagnetic coupling ($J < 0$)

For comparison we plot the coefficients α_0'' and β_0'' for $J = -0.1$, i.e. the case of ferromagnetic coupling in Fig.7a,b. For the ferromagnetic coupling we do not observe the two maxima as in the Kondo case. Furthermore, the coefficients have negative sign in half of the energy range, reducing the

amplitudes of the AFR states at $r = 0$, the position of the d^* -moment.

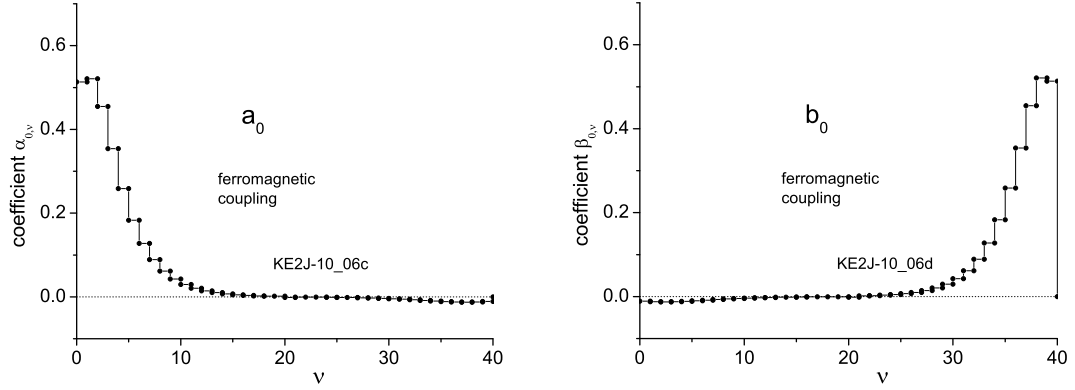


Fig.7a,b: The coefficients of the AFR states α'_0 and β'_0 as a function of ν for the two AFR states a_0^* and b_0^* . The exchange interaction is ferromagnetically coupling ($J = -0.1$).

4 Discussion

Yosida [23] introduced in the 1960's an approximate solution for the Kondo Hamiltonian of the form

$$\Psi = \frac{1}{\sqrt{2}} (a_{0\uparrow}^* d_{\downarrow}^* + d_{\uparrow}^* a_{0\downarrow}^*) |0\rangle$$

where

$$|0\rangle = \prod_{\substack{\sigma, \mathbf{k} \\ k < k_F}} c_{\mathbf{k}, \sigma}^* \Phi_0$$

is the quasi-vacuum with all states $c_{\mathbf{k}}^*$ below the Fermi energy occupied and a_0^* is an optimized single electron state which is composed of states with $k > k_F$. The state a_0^* is therefore orthogonal to all occupied states. Φ_0 is the vacuum state. Yoshida's ground-state energy and singlet-triplet energy were of the same order of magnitude with

$$E_{00} = D \exp\left(-\frac{1}{\frac{3}{2}J\rho}\right)$$

Yosida's ansatz and our suggested AFR ground state are related to each other in many respects: (i) Both use a localized state a_0^* , (ii) both form pair states between the localized state and the d^* state with zero spin component in z-direction, (iii) both fill the remaining electrons into states which are orthogonal to a_0^* . The main difference is that in our approach the state a_0^* together with a second state b_0^* are composed of all band states. This requires the remaining electron states to be aligned perpendicular to the localized states. Our AFR ground state is in a way a revival of Yosida's approach.

4.0.3 Ferromagnetic versus anti-ferromagnetic coupling

The numerical calculations show that the ground state for the anti-ferromagnetic ($J > 0$, Kondo effect) and the ferromagnetic coupling ($J < 0$) are very different.

- The ground-state energy for positive J lies lower. The behavior is roughly described by the two fits to the numerical results:
 - For $J > 0$: $E_{0+} = -.5017 * J^2 + .435 * J^3 - 9.65 * J^4$
 - For $J < 0$: $E_{0-} = -.4630 * |J|^2 + .680 * |J|^3 - .697 * |J|^4$
- There is essentially no singlet-triplet excitation energy in the case of ferromagnetic coupling. The reason is that the system adjusts in such a way that not only the states with opposite d^* -state spin (for example ψ_B and ψ_C) are orthogonal but even the states with the same d^* -state spin orientation (for example ψ_B and $\psi_{\overline{C}}$) are quasi-orthogonal. This becomes visible in the (multi-electron) scalar products between the state $\psi_B, \psi_{\overline{C}}, \psi_C, \psi_{\overline{B}}$. For $J = -0.1$ the scalar products $\langle \psi_B | \psi_{\overline{C}} \rangle$ and $\langle \psi_C | \psi_{\overline{B}} \rangle$ are of the order of 10^{-6} while in the anti-ferromagnetic Kondo ($J = 0.1$) $\langle \psi_B | \psi_{\overline{C}} \rangle$ and $\langle \psi_C | \psi_{\overline{B}} \rangle$ are of the order of $1/3$. In the case of the ferromagnetic coupling $J < 0$ the two bases $\{a_0^*, a_i^*\}$ and $\{b_0^*, b_i^*\}$ align themselves in such a way that the scalar product between $|0_a\rangle$ and $|0_b\rangle$ with n occupied states is of the order of $\langle 0_a | 0_b \rangle \approx 10^{-3}$. The bases align themselves quasi-orthogonal. Therefore the reduction of the ground-state energy is solely due to z-component of the interaction. The energy matrix element of the x-y-component of the interaction is practically zero.

4.0.4 Coefficients of the ground- and excited state

Our Kondo-ground state ψ_K is given by (7). The coefficient-vector $(V) = (B \ \overline{C} \ C \ \overline{B})^\dagger$ contains interesting information about the structure of the states. Here we discuss the results for $J = 0.1$, $N = 40$. In the ground state $(V)^\dagger$ takes the values $(V)^\dagger_{\text{ground}} = (.703, .0626, .0626, .703)$ and in the excited state we find $(V)^\dagger_{\text{excited}} = (.705, -.0635, .0635, -.705)$. (Note that state $\psi_{K,0}$ and $\psi_{K,1}$ are normalized but not the vectors (V) because the pairs of states $\psi_B, \psi_{\overline{C}}$ and $\psi_C, \psi_{\overline{B}}$ are not orthogonal as discussed in the appendix). For both, ground and excited states, the sub-states with a_0^* have a large amplitude while the sub-states with the state b_0^* have a small amplitude. In the ground state all coefficients are positive. In the excited state the sub-states with opposite d^* -spin have opposite sign. These are the signatures of a singlet ground state and triplet excited state. (Note that the states are ordered according to their spin).

For the ferromagnetic coupling we obtain for $J = -0.1$, $N = 40$ the following coefficients: In the ground state $(V)^\dagger$ takes the values $(V)^\dagger_{\text{ground}} = (-.706, -.0400, .0400, .706)$. For the essentially degenerated excited state we find $(V)^\dagger_{\text{excited}} = (.706, -.0400, -.0400, .706)$. This means that in the ground state the components with $Ba_{0\uparrow}^*d_{\downarrow}^*$ and $\overline{B}d_{\uparrow}^*a_{0\downarrow}^*$ form a triplet state (as do the components $Cd_{\uparrow}^*b_{0\downarrow}^*$ and $\overline{C}b_{0\uparrow}^*d_{\downarrow}^*$) but the signs of the states which contain a_0^* and b_0^* with the same spin are opposite.

4.0.5 Singlet-triplet excitation energy

The triplet state $\psi_{K,1}$ is obtained by minimizing the ground-state energy. Then $\psi_{K,1}$ is the first excited state. This state $\psi_{K,1}$ is composed of the same Slater states $\psi_B, \psi_C, \psi_{\overline{B}}, \psi_{\overline{C}}$ as the singlet state. Only the coefficients, and particularly their signs, are different than in $\psi_{K,0}$. But this state is not necessarily the triplet state with the lowest energy. To obtain the lowest triplet state during the minimization we impose on the coefficients B, C and $\overline{B}, \overline{C}$ the conditions

$$\overline{B} = -B \quad \overline{C} = -C$$

This automatically enforces the triplet state. With these conditions we repeat the optimization procedure to obtain the lowest triplet energy. The resulting state is a relaxed triplet state. We denote it as $\overline{\psi}_{K,1}$. Its Slater states $\overline{\psi}_B, \overline{\psi}_C, \overline{\psi}_{\overline{B}}, \overline{\psi}_{\overline{C}}$ are different than for the singlet ground state $\psi_{K,0}$. Its energy $\overline{E}_{K,1}$ is lower than the energy $E_{K,1}$ of the unrelaxed triplet state $\psi_{K,1}$.

Now we can take the energy difference between the energy of the relaxed triplet state and the singlet state. Because the two values are obtained in two different optimization calculations the absolute accuracy of the optimization has to be better than 10^{-10} (in units of the band width). We plot the new excitation energy in Fig.2 as stars. It lies below the unrelaxed excitation energy. The latter is approximately given by $\Delta E_{st} \approx 5D \exp[-1/(2J\rho_0)]$. Our new values for the excitation energy lie between two theoretical curves: (i) $\Delta E_{st} = D \exp[-1/(2J\rho_0)]$, given by the dashed curve and (ii) $\Delta E_{st} = \sqrt{2J\rho_0}D \exp[-1/(2J\rho_0)]$, given by the dotted curve. Both expressions are given in the literature as approximate values for the Kondo temperature $k_B T_K$. The numerical values lie closer to the second expression.

4.1 The artificial Friedel resonance states

In the Fig.5a,b and 7a,b the coefficients α_0^ν (or β_0^ν respectively) as they occur in equ. (8) are plotted as a function of ν . One has to recall that for $N = 40$ the Fermi energy lies in the center at $\nu = 20$. The energies above the Fermi energy are: $\frac{1}{2}2^{-19}, \frac{3}{2}2^{-19}, \frac{3}{2}2^{-18}, \dots, \frac{3}{2}2^{-1}$. The energy states below the Fermi energy are a mirror image of the state above.

The Kondo and the ferromagnetic case have in common that the coefficients of a_0^* and b_0^* are almost mirror images. The state a_0^* has its main weight at negative energies and b_0^* at positive energies.

Beyond that the ferromagnetic and anti-ferromagnetic cases differ considerably. The coefficients in the Kondo case are all positive whereas in the ferromagnetic case the signs in the positive and negative energy regimes are different.

5 Conclusion

In this paper we have developed a compact (approximate) ground state for the Kondo problem. Two localized s-electron states, a_0^* and b_0^* are built from the s-band. Their amplitudes, normally two times 40 numbers, determine fully the ground state. This ground state consists of four Slater determinants. It yields two energies, the total ground-state energy E_{00} and the singlet-triplet excitation energy ΔE_{st} . While E_{00} depends essentially quadratically on the coupling constant J , the energy ΔE_{st} shows an exponential dependence. It

is given by

$$\Delta E_{st} \approx 5 * \exp \left(-\frac{1}{2J\rho} \right)$$

and is proportional to the Kondo temperature.

The energy scales of ΔE_{st} and E_{00} are very far apart. They differ by a factor 100 to 1000. It is remarkable that our solution works for both energy ranges at the same time.

Our ansatz shows also a very different solution for the Kondo ($J > 0$) case than for the ferromagnetically coupled case ($J < 0$). In particular the latter has no singlet-triplet splitting, and the different sub-states ψ_X avoid each other by forming quasi-orthogonal multi-electron states.

The structures of the localized AFR states α_0^* and b_0^* differ considerably between the $J > 0$ and the $J < 0$ case. In particular for the $J > 0$ case the coefficients have two maxima in an intermediate positive and negative energy range. A better understanding of these structures is left for future investigations.

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A Appendix

A.1 Wilson's s-electron basis

Wilson [5] in his Kondo paper considered an s-band with energy values ranging from -1 to 1 . In the next step Wilson replaced the continuum of s-states by a discrete set of states. This is done on a logarithmic scale. The discrete energy values are $1, 1/\Lambda, 1/\Lambda^2$, etc and $-1, -1/\Lambda, -1/\Lambda^2$, etc where Λ is a parameter larger than one. (In this paper $\Lambda = 2$ is chosen). These discrete ξ_ν points are used to define a sequence of intervals: the interval ν (for $\nu < N/2$) is $\xi_{\nu-1} = -1/2^{\nu-1} < \varepsilon < -1/2^\nu = \xi_\nu$ (there are equivalent intervals for positive ξ -values where ν is replaced by $(N - \nu)$ but we discuss here only the negative energies). The new Wilson states c_ν^* are a superposition of all states in the energy interval $(\xi_{\nu-1}, \xi_\nu)$ and have an (averaged) energy $(\xi_\nu + \xi_{\nu-1})/2 = \left(-\frac{3}{2}\right) \frac{1}{2^\nu}$, i.e. $-\frac{3}{4}, -\frac{3}{8}, -\frac{3}{16}, \dots, -\frac{3}{2 \cdot 2^{N/2}}, -\frac{1}{2 \cdot 2^{N/2}}$. This spectrum continues symmetrically for positive energies. The essential advantage of the Wilson basis is that it has an arbitrarily fine energy spacing at the Fermi energy.

While Wilson chose the logarithmic energy scale for his scaling approach, in this paper the physical background is somewhat different. We start (like Wilson) with the somewhat artificial energy band in the range $(-1, 1)$ which has a constant density of states. The volume of the host is V_h and the atomic volume v_A . The full band (per spin) shall have one electron per atomic volume. So the total number of electrons of a full band in the volume V_h is $Z = V_h/v_A$. The electron density per spin of a full band is $n = Z/V_h = 1/v_A$. The density of states (per spin) is $Z/2$ in the volume V_h and equal to $\rho = 1/2$ in the volume v_A .

In this model the original energy levels have a (constant) separation of $\delta E = 2v_A/V_h$ which will be in the range between 10^{-8} to 10^{-23} . In an energy interval $(\xi_{\nu-1}, \xi_\nu)$ one has a large number Z_ν of electron states $\varphi_\mu(r)$ with $1 \leq \mu \leq Z_\nu$. Their level separation shall be constant and the value of the wave function at the origin $\varphi_\mu(0) = 1/\sqrt{V_h}$ is independent of μ .

Next we form a new basis $\chi_\alpha(r)$ for the energy range $(\xi_\nu, \xi_{\nu-1})$. We renumber all the original states $\varphi_\mu(\mathbf{r})$ in this energy range from 1 to Z_ν and define the new state (or wave function) $\chi_\alpha(\mathbf{r})$ ($1 \leq \alpha \leq Z_\nu$)

$$\chi_\alpha(\mathbf{r}) = \frac{1}{\sqrt{Z_\nu}} \sum_{\mu=1}^{Z_\nu} \varphi_\mu(\mathbf{r}) e^{i2\pi\alpha\mu/Z_\nu}$$

In the new basis $\chi_\alpha(\mathbf{r})$ all states except $\chi_{Z_\nu}(r)$ have a zero amplitude at the origin.

$$\chi_\alpha(0) = \left\{ \begin{array}{ll} = 0 & \text{for } 1 \leq \alpha < Z_\nu \\ \sqrt{\frac{Z_\nu}{V_h}} & \text{for } \alpha = Z_\nu \end{array} \right|$$

In the following we denote the state χ_{Z_ν} as ψ_ν and neglect all other $\chi_\alpha(\mathbf{r})$ -states because the latter do not interact with the impurity. The field operator $\Psi(\mathbf{r})$ in the original basis φ_μ has the form (c_{φ_μ} is the annihilation operator for the state $\varphi_\nu(\mathbf{r})$)

$$\Psi(\mathbf{r}) = \sum_{\mu=1}^Z \varphi_\mu(\mathbf{r}) c_{\varphi_\mu}$$

We can divide $\Psi(\mathbf{r})$ into one part which is non-zero at $\mathbf{r} = \mathbf{0}$ and a second part which vanishes at zero. For the interaction with the d-impurity only the first part contributes. This part is equal to

$$\bar{\Psi}(\mathbf{r}) = \sum_\nu \psi_\nu(\mathbf{r}) c_\nu$$

At $\mathbf{r} = \mathbf{0}$ one has

$$\begin{aligned} \Psi(\mathbf{0}) &= \bar{\Psi}(\mathbf{0}) = \sum \psi_\nu(\mathbf{0}) c_\nu = \sum \sqrt{\frac{Z_\nu}{V_h}} c_\nu \\ &= \frac{1}{\sqrt{v_a}} \sum \sqrt{\frac{Z_\nu}{Z}} c_\nu = \frac{1}{\sqrt{v_a}} \sum \sqrt{\frac{\Delta \zeta_\nu}{2}} c_\nu \end{aligned}$$

The width of the energy ranges can be chosen arbitrarily. We use Wilson's exponential energy spectrum. This resulting basis $\{c_\nu^*\}$ is the starting point for all calculations.

Since J is the matrix element per atomic volume we have to use also the density of states per atomic volume. The latter is

$$\rho = \frac{1}{2}$$

A.2 Construction of the Basis a_0^*, a_i^*

For the construction of the state a_0^* and the rest of basis a_i^* one starts with the s-band electrons $\{c_\nu^*\}$ which consist of N states (for example Wilson's states). The d^* -state is ignored for the moment.

- In step (1) one forms a normalized state a_0^* out of the s-states with:

$$a_0^* = \sum_{\nu=1}^N \alpha_\nu^0 c_\nu^* \quad (10)$$

The coefficients α_ν^0 can be arbitrary at first. One reasonable choice is $\alpha_\nu^0 = 1/\sqrt{N}$

- In step (2) $(N - 1)$ new basis states \bar{a}_i^* ($1 \leq i \leq N - 1$) are formed which are normalized and orthogonal to each other and to a_0^* .
- In step (3) the s-band Hamiltonian H_0 is constructed in this new basis. One puts the state a_0^* at the top so that its matrix elements are H_{0i} and H_{i0} .
- In step (4) the $(N - 1)$ -sub Hamiltonian which does not contain the state a_0^* is diagonalized. This transforms the rest of the basis $\{\bar{a}_i^*\}$ into a new basis $\{a_i^*, a_i^*\}$ (but keeps the state a_0^* unchanged). The resulting Hamilton matrix for the s-band then has the form

$$H_0 = \begin{pmatrix} E(0) & V_{fr}(1) & V_{fr}(2) & \dots & V_{fr}(N-1) \\ V_{fr}(1) & E(1) & 0 & \dots & 0 \\ V_{fr}(2) & 0 & E(2) & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ V_{fr}(N-1) & 0 & 0 & \dots & E(N-1) \end{pmatrix} \quad (11)$$

The creation operators of the new basis are given by the set $\{a_0^*, a_i^*\}$, ($0 < i \leq N - 1$). The a_i^* can be expressed in terms of the s-states; $a_i^* = \sum_{\nu=1}^N \alpha_\nu^i c_\nu^*$. The state a_0^* uniquely determines the other states a_i^* . The state a_0^* is coupled through the matrix elements $V_{fr}(i)$ to the states a_i^* , which makes the state a_0^* an artificial Friedel resonance. The matrix elements $E(i)$ and $V_{fr}(i)$ are given as

$$E(i) = \sum_{\nu} \alpha_\nu^i \varepsilon_\nu \alpha_\nu^i$$

$$V_{fr}(i) = \sum_{\nu} \alpha_\nu^0 \varepsilon_\nu \alpha_\nu^i$$

- In the final step (5) the state a_0^* is rotated in the N -dimensional Hilbert space. In each cycle the state a_0^* is rotated in the $(a_0^*, a_{i_0}^*)$ plane by an angle θ_{i_0} for $1 \leq i_0 \leq N - 1$. Each rotation by θ_{i_0} yields a new \bar{a}_0^*

$$\bar{a}_0^* = a_0^* \cos \theta_{i_0} + a_{i_0}^* \sin \theta_{i_0}$$

The rotation leaves the whole basis $\{a_0^*, a_i^*\}$ orthonormal. Step (4), the diagonalization of the $(N - 1)$ -sub Hamiltonian, is now much quicker because the $(N - 1)$ -sub-hamiltonian is already diagonal with the exception of the i_0 - row and the i_0 -column . For each rotation plane $(a_0^*, a_{i_0}^*)$ the optimal a_0^* with the lowest energy expectation value is determined. This cycle is repeated until one reaches the absolute minimum of the energy expectation value. In the example of the Friedel resonance Hamiltonian this energy agrees numerically with an accuracy of 10^{-15} with the exact ground-state energy of the Friedel Hamiltonian [20]. For the Kondo impurity the procedure is stopped when the expectation value changes by less than 10^{-10} during a full cycle.

A.3 Matrix elements

In equ.(5) we expressed the Kondo Hamiltonian in terms of field operators. We can also express it in the basis $\{c_\nu^*\}$. Here it has the form

$$H_{sd} = \sum_{\nu, \nu'} J_{\nu, \nu'} \left(S_+ c_{\nu\downarrow}^\dagger(0) c_{\nu'\uparrow}(0) + S_- c_{\nu\uparrow}^\dagger(0) c_{\nu'\downarrow}(0) \right) + S_z \left(c_{\nu\uparrow}^\dagger(0) c_{\nu'\uparrow}(0) - c_{\nu\downarrow}^\dagger(0) c_{\nu'\downarrow}(0) \right)$$

with

$$J_{\nu, \nu'} = J \sqrt{\frac{\Delta\zeta_\nu}{2}} \sqrt{\frac{\Delta\zeta_{\nu'}}{2}}, \quad \Delta\zeta_\nu = \zeta_\nu - \zeta_{\nu-1}$$

We will, however, use (a slightly modified version of) equ.(5). The non-spin-flip part can be rewritten as

$$H_{nsf} = v_a J S_z \left(-\Psi_\uparrow(0) \Psi_\uparrow^\dagger(0) + \Psi_\downarrow(0) \Psi_\downarrow^\dagger(0) \right) \quad (12)$$

where we anti-commuted the field operators.

We consider first the example of the non-spin-flip part where the spin of

the d-impurity and the s-electrons are anti-parallel:

$$\begin{aligned}
\langle \psi_B | H_{\uparrow\uparrow} | \psi_B \rangle &= -v_a J \left\langle a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \left| S_z \Psi_{\uparrow}(0) \Psi_{\uparrow}^{\dagger}(0) \right| a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \right\rangle \\
&= \frac{v_a J}{2} \left\langle a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \left| \Psi_{\uparrow}(0) \Psi_{\uparrow}^{\dagger}(0) \right| a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \right\rangle \\
&= \frac{v_a J}{2} \left\langle \Psi_{\uparrow}(0) a_{0\uparrow}^* \mathbf{0}_{a\uparrow} d_{\downarrow}^* \mathbf{0}_{b\downarrow} \parallel \Psi_{\uparrow}^{\dagger}(0) a_{0\uparrow}^* \mathbf{0}_{a\uparrow} d_{\downarrow}^* \mathbf{0}_{b\downarrow} \right\rangle \\
&= \frac{v_a J}{2} \sum_{i=0}^n |A_i^a|^2
\end{aligned}$$

where A_i^a is the amplitude of the state a_i^* at $r = 0$. The summation is from $0 \leq i \leq n$. Similarly one obtains for the non-spin-flip part where the spin of the d-impurity and the s-electrons are parallel:

$$\langle \psi_B | H_{\downarrow\downarrow} | \psi_B \rangle = v_a J \left\langle a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \left| J S_z \Psi_{\downarrow}(0) \Psi_{\downarrow}^{\dagger}(0) \right| a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \right\rangle = -\frac{v_a J}{2} \sum_{i=1}^n |A_i^b|^2$$

A_i^b is the amplitude of the state b_i^* at the origin. The latter summation is from $1 \leq i \leq n$.

As an example for the spin-flip matrices one obtains

$$\begin{aligned}
\langle \psi_{\overline{B}} | H_{\uparrow\downarrow} | \psi_B \rangle &= v_a J \left\langle d_{\uparrow}^* a_{0\downarrow}^* \mathbf{0}_{b\uparrow} \mathbf{0}_{a\downarrow} \left| S_+ \Psi_{\downarrow}^{\dagger}(0) \Psi_{\uparrow}(0) \right| a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \right\rangle \\
&= -v_a J \left\langle \Psi_{\uparrow}^{\dagger}(0) d_{\uparrow}^* a_{0\downarrow}^* \mathbf{0}_{b\uparrow} \mathbf{0}_{a\downarrow} \parallel \Psi_{\downarrow}^{\dagger}(0) a_{0\uparrow}^* d_{\downarrow}^* \mathbf{0}_{a\uparrow} \mathbf{0}_{b\downarrow} \right\rangle \\
&= -v_a J \left\langle \Psi_{\uparrow}^{\dagger}(0) \mathbf{0}_{b\uparrow} a_{0\downarrow}^* \mathbf{0}_{a\downarrow} \parallel a_{0\uparrow}^* \mathbf{0}_{a\uparrow} \Psi_{\downarrow}^{\dagger}(0) \mathbf{0}_{b\downarrow} \right\rangle \\
&= -v_a J \left\langle a_{0\downarrow}^* \mathbf{0}_{a\downarrow} \parallel \Psi_{\downarrow}^{\dagger}(0) \mathbf{0}_{b\downarrow} \right\rangle \left\langle \Psi_{\uparrow}^{\dagger}(0) \mathbf{0}_{b\uparrow} \parallel a_{0\uparrow}^* \mathbf{0}_{a\uparrow} \right\rangle \\
&= -v_a J \left| \langle \Psi_{\uparrow}^{\dagger}(0) \mathbf{0}_b \parallel a_{0\uparrow}^* \mathbf{0}_a \rangle \right|^2
\end{aligned}$$

The final brackets $\langle \rangle$ represent a multi-scalar product which is given by the determinant of the following $(n+1) \times (n+1)$ matrix.

$$\begin{aligned}
&\langle \Psi_{\uparrow}^{\dagger}(0) \mathbf{0}_b \parallel a_{0\uparrow}^* \mathbf{0}_a \rangle \\
&= \begin{vmatrix} \langle \Psi^*(0) | a_0^* \rangle & \langle \Psi^*(0) | a_1^* \rangle & \langle \Psi^*(0) | a_n^* \rangle \\ \langle b_1^* | a_0^* \rangle & \langle b_1^* | a_1^* \rangle & \langle b_1^* | a_n^* \rangle \\ \langle b_n^* | a_0^* \rangle & \langle b_n^* | a_1^* \rangle & \langle b_n^* | a_n^* \rangle \end{vmatrix}
\end{aligned}$$

$$= \begin{vmatrix} A_0^a & A_1^a & \dots & A_n^a \\ \langle b_1^* | a_0^* \rangle & \langle b_1^* | a_1^* \rangle & \dots & \langle b_1^* | a_n^* \rangle \\ \dots & \dots & \dots & \dots \\ \langle b_n^* | a_0^* \rangle & \langle b_n^* | a_1^* \rangle & \dots & \langle b_n^* | a_n^* \rangle \end{vmatrix}$$

A.4 Energy optimization

For a given set of bases $\{a_0^*, a_i^*\}$ and $\{b_0^*, b_i^*\}$ the energy expectation value of the Kondo state is given by

$$\langle E \rangle = \frac{\langle \psi_K | H | \psi_K \rangle}{\langle \psi_K | \psi_K \rangle}$$

The numerator of the expectation value of the ground-state energy is given by

$$\langle \psi_K | H | \psi_K \rangle = \begin{pmatrix} B & \overline{C} & C & \overline{B} \end{pmatrix} \begin{pmatrix} H_{BB} & H_{B\overline{C}} & H_{BC} & H_{B\overline{B}} \\ H_{\overline{C}B} & H_{\overline{C}\overline{C}} & H_{\overline{C}C} & H_{\overline{C}\overline{B}} \\ H_{CB} & H_{C\overline{C}} & H_{CC} & H_{C\overline{B}} \\ H_{\overline{B}B} & H_{\overline{B}\overline{C}} & H_{\overline{B}C} & H_{\overline{B}\overline{B}} \end{pmatrix} \begin{pmatrix} B \\ \overline{C} \\ C \\ \overline{B} \end{pmatrix} \quad (13)$$

where $(V) = \begin{pmatrix} B & \overline{C} & C & \overline{B} \end{pmatrix}^\dagger$. The denominator is given by

$$\langle \psi_K | \psi_K \rangle = (V)^\dagger (N) (V)$$

where (N) is the non-diagonal symmetric matrix of the scalar products $\langle \psi_X | \psi_Y \rangle$ (since the Slater states ψ_X are pair-wise not orthogonal)

$$(N) = \begin{pmatrix} 1 & \langle \psi_B | \psi_{\overline{C}} \rangle & 0 & 0 \\ \langle \psi_{\overline{C}} | \psi_B \rangle & 1 & 0 & 0 \\ 0 & 0 & 1 & \langle \psi_C | \psi_{\overline{B}} \rangle \\ 0 & 0 & \langle \psi_{\overline{B}} | \psi_C \rangle & 1 \end{pmatrix}$$

With an orthogonal transformation of (V) the matrix (N) can be transformed into a diagonal matrix $(\overline{N}) = (N_{ii} \delta_{ij})$. Replacing $V_i \rightarrow V_i / \sqrt{N_{ii}}$ transforms the matrix (N) into the unity matrix.

Now we can require that the new vector (V') is normalized so that $\langle \psi_K | \psi_K \rangle = (B'^2 + \overline{C}'^2 + C'^2 + \overline{B}'^2) = 1$ and we have only to vary the numerator. This yields the eigenvalue problem

$$(H') (V') = \Lambda (V') \quad (14)$$

which can be easily solved numerically. The original coefficients $(B \ \overline{C} \ C \ \overline{B})$ are obtained by reversing the transformations.

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